Local spin polarization in underdoped cuprates with impurities

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We present a theory of magnetic (Ni) and nonmagnetic (Zn) impurities substituted into planar Cu sites in the normal state of underdoped cuprates exhibiting a spin gap. Both types of impurities induce magnetic moments on neighboring Cu sites. In the case of Ni these moments partially screen the inherent impurity spin, resulting in an effective $S = 1/2$ moment. The characteristic Kondo scale is found to have a power-law dependence on the coupling constant. We investigate the spatial shape of the impurity-induced spin density, taking into account the presence of short-ranged AF correlations, and calculate the ^{17}O NMR line broadening induced by impurity doping.

The most striking features observed in the normal state of underdoped cuprates are the occurance of a magnetic pseudogap and the persistence of antiferromagnetic (AF) correlations in the metallic state. Experimentally, the local magnetic properties of the cuprates can be sensitively probed by introducing impurities into the magnetically active Cu sites of the CuO_2 planes and by subsequently measuring the effect on the NMR signal of nuclei coupled to the planes.

Magnetic Ni (d^8) and nonmagnetic Zn (d^{10}) substituting for Cu (d^9) are both found to introduce magnetic moments into the planes. Measurements of the macroscopic susceptibility show an almost perfect $1/T$ Curie behavior, the moments being stronger for Ni than for Zn [1]. Recently, Bobroff et al. [2] presented novel ^{17}O NMR measurements for $YBa_2(Cu_{1-x}(Zn/Ni)_x)_3O_{6.6}$ probing the long-range polarization of the CuO_2 planes. In contrast to the aforementioned bulk experiment, Zn had a larger impact on the NMR line width than Ni, indicating a very different spatial variation of the polarization induced by the two types of impurities. Furthermore, a markable deviation from the expected $1/T$ behavior of the line broadening was observed, which was interpreted by Morr et al. [3] as an indication of a temperature dependence of the AF correlation length ξ. Here we present a microscopic theory of the impurity-induced local spin polarization in underdoped cuprates. We show that the presence of the spin gap and of short-range AF correlations strongly modifies the conventional RKKY picture which explains the peculiarities in NMR line broadening data.

The planar Cu spins are described by a Heisenberg model treated in resonance valence bond (RVB) mean-field theory

$$H_{\rm RVB} = -\sum_{\langle ij\rangle,\sigma}\left(\Delta_{ij} f^\dagger_{i\sigma} f_{j\sigma} + \text{H.c.}\right). \qquad (1)$$

Dividing the lattice into two sublattices, the symmetry of the order parameter Δ_{ij} is chosen such as to obtain a pseudogap in the magnetic excitation spectrum [4] with density of states $\rho(\omega) = |\omega|/D^2$, where D is the spinon bandwidth; implicitly we assume this magnetic gap to be stabilized by the motion of holes present in the doped system. Magnetic and nonmagnetic impurities at site 0 are modelled by

$$H_{\rm Ni} = H'_{\rm RVB} + J' \sum_\delta \boldsymbol{s}_\delta \cdot \boldsymbol{S}_0, \qquad (2)$$

$$H_{\rm Zn} = H_{\rm RVB} + \lambda f^\dagger_0 f_0|_{\lambda\to\infty}, \qquad (3)$$

respectively, where $\boldsymbol{S}_0$ is the spin of Ni and $\boldsymbol{s}_\delta$ that of its nearest neighbor Cu sites, and $H'_{\rm RVB}$ is obtained from Eq. (1) by excluding site 0 from the sum over bonds. The $S = 1$ Ni spin is represented by two ferromagnetically coupled $S = 1/2$ spins with coupling constant $|J_c| \gg |J'|$.

In the spin gap phase, Ni and Zn both induce moments on the Cu sites in the vicinity of the impurity [5]. In the case of Ni, these moments themselves partially screen the inherent spin of Ni, resulting in an effective $S = 1/2$ moment localized on the Ni site. The situation resembles that of an underscreened Kondo problem; the Kondo energy $\omega_k \propto J'/\ln J'$ is, however, found to exhibit a power-law rather than the usual exponential dependence on the coupling parameter J' stemming from the fact that the Ni spin couples predominantly to the spinon bound state but not to extended states. The formation of the Kondo state renormalizes the magnetic gap but does not fill it. The low-energy fixed point of the system is therefore that of an external $S = 1/2$ spin coupled ferromagnetically to an impurity-free spin lattice with renormalized gap. The impurity-induced long-range polarization of the planar spins is $K_{\rm Ni}(\boldsymbol{R}, T) \propto R^{-3}T^{-1}$ for $\boldsymbol{R}$ pointing to the sublattice not containing the impurity, while it is found to be negligible otherwise. We notice that the rapid ($\propto R^{-3}$) decay, which should be compared to the conventional Ruderman-Kittel polarization in two dimensions ($\propto R^{-2}$), is due to the presence of the spin pseudogap, a feature which is robust against Ni doping.

In the case of Zn which carries no internal spin, the moments induced in the neighborhood of the impurity are not screened. The moment associated with Zn is there-

fore only weakly localized, resulting in a slower spatial decay of the polarizability $K_{\rm Zn}(\boldsymbol{R},T) \propto R^{-2}(T\ln(D/T))^{-1}$ as compared to Ni; for $\boldsymbol{R}$ pointing to the impurity sublattice, $K_{\rm Zn}(\boldsymbol{R},T)$ is negligible.

The broadening $\Delta\nu$ of the NMR line of a given planar ^{17}O is dominated by the polarization of the two neighboring Cu sites. Since $K(\boldsymbol{R},T)$ decays more slowly with distance for Zn than for Ni one expects $\Delta\nu_{\rm Zn} > \Delta\nu_{\rm Ni}$ for small impurity concentration which is in agreement with experiment. However, the non-Curie behavior of $\Delta\nu$ observed by Bobroff et al. is not yet captured in the expressions for $K(\boldsymbol{R},T)$. We therefore extend our theory to include short-range AF correlations underestimated in the above mean-field treatment. Within a random-phase approximation (RPA) one finds $K_{\rm RPA}(\boldsymbol{q},T) = K(\boldsymbol{q},T)S_{\boldsymbol{q}}(T)$ with the Stoner enhancement factor

$$S_{\boldsymbol{q}}(T) = \frac{\xi^2(T)}{1+(\boldsymbol{q}-\boldsymbol{Q})^2\xi^2(T)} \tag{4}$$

for momenta $\boldsymbol{q}$ close to $\boldsymbol{Q}=(\pi,\pi)$. At large enough distance the polarization induced by Ni or Zn, respectively, is

$$K_{\rm Ni}(\boldsymbol{R},T) = \pm\frac{3}{2\pi^3}\frac{1}{R^3}\frac{\xi^2(T)}{T}, \tag{5}$$

$$K_{\rm Zn}(\boldsymbol{R},T) = \pm\frac{1}{8\pi}\frac{1}{R^2}\frac{\xi^2(T)}{T\ln(D/T)}, \tag{6}$$

where the alternating sign refers to the two different sublattices. The NMR frequency shift induced by a given impurity at position $\boldsymbol{R}$ relative to a ^{17}O nucleus is

$$\Delta\omega = \gamma_e A_{\rm hf} H\left[K(\boldsymbol{R}-\boldsymbol{\delta}/2,T)+K(\boldsymbol{R}+\boldsymbol{\delta}/2,T)\right], \tag{7}$$

where $A_{\rm hf}$ is the n.n. hyperfine coupling constant, γ_e the electronic magnetogyric ratio, H the external magnetic field, and $\boldsymbol{\delta}$ a lattice vector. Due to the alternating sign of the polarizability and the fact that each ^{17}O nucleus lies in between two different sublattices, the term in brackets in Eq. (7) partially vanishes; thus effectively the spatial derivative of $K(\boldsymbol{R},T)$ is probed by NMR. The impurity-induced line broadening is finally calculated from Eqs. (5), (6), and (7) employing the formalism given in [6] to average over random impurity configurations, yielding

$$\Delta\nu_{\rm Ni} \approx 1.32\gamma_e A_{\rm hf} H x^2 \frac{\xi^2(T)}{T}, \tag{8}$$

$$\Delta\nu_{\rm Zn} \approx 0.77\gamma_e A_{\rm hf} H x^{3/2} \frac{\xi^2(T)}{T\ln(D/T)} \tag{9}$$

with impurity concentration x.

We assume a phenomenological form $\xi(T) = 1/(a+bT)$ for the AF correlation length [7], where a and b are fitting parameters of our theory. In Fig. 1 the result for $T\Delta\nu$ is compared to experimental ^{17}O NMR data. We choose

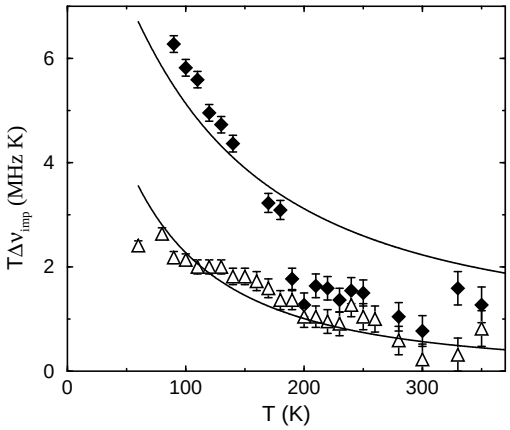

FIG. 1. Impurity-induced line broadening $T\Delta\nu$. The theoretical result is indicated by solid lines fitted to ^{17}O NMR data for 1% Ni-doped (triangles) and 1% Zn-doped (diamonds) $YBa_2(Cu_{1-x}(Zn/Ni)_x)_3O_{6.6}$ [2].

$a = 0.07$ and $b = 0.0007$ corresponding to $\xi = 4.8$ in units of lattice spacings at $T = 200$ K, which compares to $\xi = 5.9$ obtained in [8]. We note that saturation of the AF correlation length which is expected to occur at low temperatures is not yet included in the phenomenological expression used for $\xi(T)$.

In conclusion, we have presented a theory of magnetic and nonmagnetic impurities in the normal state of underdoped cuprates. Based on the existence of a spin gap and extended to account for the presence of AF correlations the theory gives a description of the different magnetic behavior of Ni and Zn impurities and explains well recent experimental results for the impurity-induced ^{17}O NMR line broadening.

[1] P. Mendels et al., Physica C 235-240 (1994) 1595.

[2] J. Bobroff et al., Phys. Rev. Lett. 79 (1997) 2117; Physica C 282-287 (1997) 1389.

[3] D. K. Morr, J. Schmalian, R. Stern, C. P. Slichter, Phys. Rev. Lett. 80 (1998) 3662; preprint cond-mat/9801317.

[4] I. Affleck, J. B. Marston, Phys. Rev. B 37 (1988) 3774; Y. Suzumura, Y. Hasegawa, H. Fukuyama, J. Phys. Soc. Jpn. 57 (1988) 2768; G. Kotliar, Phys. Rev. B 37 (1988) 3664.

[5] G. Khaliullin, R. Kilian, S. Krivenko, P. Fulde, Phys. Rev. B 56 (1997) 11 882; Physica C 282-287 (1997) 1749.

[6] R. E. Walstedt and L. R. Walker, Phys. Rev. B 9 (1974) 4857.

[7] B. P. Stojković and D. Pines, Phys. Rev. B 56 (1997) 11 931.

[8] V. Barzykin and D. Pines, Phys. Rev. B 52 (1995) 13 585.